

W0029

CrystMol 2.1 – New Tools for Analysis of Multiple Determinations of the Same or Similar Structures. David J. Duchamp, Kalamazoo, MI 49009.

A new molecular overlay module has been added to CrystMol to facilitate comparison of multiple experimental determinations of the same and similar molecules. New software supports automatic (one click) overlay of multiple molecules in the asymmetric unit. Polymorphs of the same compound may be automatically matched. Two key routines form the core of the new module. One matches molecules topologically according to their bonding arrangements, and the other moves molecules as rigid bodies to find the best overlay. Manual or semi-automatic addition and deletion of match points, overlay or spread views, and reports are available. Any number of molecules may be matched and overlaid simultaneously.

CrystMol 2.0, available in Windows and Macintosh versions, is low-cost easy-to-use structure display and analysis software for teaching and research. Designed around a crystallographic theme, CrystMol allows easy handling of space group symmetry, anisotropic thermal parameters, CIF files, standard deviations, best planes, hydrogen bonding, packing displays, QuickTime movies, etc. (See <http://www.crystmol.com/>).

Examples will show how new overlay features, combined with other CrystMol tools, such as CrystMolMM molecular mechanics, can be used for in-depth analysis of experimental results. The author welcomes all suggestions on how to improve CrystMol.